

A series of trees with the first $\lfloor \frac{n-7}{2} \rfloor$ largest energies[☆]

Hai-Ying Shan^a, Jia-Yu Shao^{a,*}, Li Zhang^a, Chang-Xiang He^b

^aDepartment of Mathematics, Tongji University, Shanghai 200092, China

^bCollege of Science, University of Shanghai for Science and Technology, Shanghai, 200093, China

Abstract

The energy of a graph is defined as the sum of the absolute values of the eigenvalues of the graph. In this paper, we present a new method to compare the energies of two k -subdivision bipartite graphs on some cut edges. As the applications of this new method, we determine the first $\lfloor \frac{n-7}{2} \rfloor$ largest energy trees of order n for $n \geq 31$, and we also give a simplified proof of the conjecture on the fourth maximal energy tree.

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1. Introduction

Let G be a graph with n vertices and A be its adjacency matrix. Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of A , then the *energy* of G , denoted by $\mathbb{E}(G)$, is defined [2, 3] as $\mathbb{E}(G) = \sum_{i=1}^n |\lambda_i|$.

The characteristic polynomial $\det(xI - A)$ of the adjacency matrix A of a graph G is also called the characteristic polynomial of G , written as $\phi(G, x) = \sum_{i=0}^n a_i(G)x^{n-i}$.

In this paper, we write $b_i(G) = |a_i(G)|$, and also write

$$\tilde{\phi}(G, x) = \sum_{i=0}^n b_i(G)x^{n-i}.$$

If G is a bipartite graph, then it is well known that $\phi(G, x)$ has the form

$$\phi(G, x) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} a_{2i}(G)x^{n-2i} = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^i b_{2i}(G)x^{n-2i} \quad (1.1)$$

and thus

$$\tilde{\phi}(G, x) = \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} b_{2i}(G)x^{n-2i}. \quad (b_{2i}(G) = |a_{2i}(G)| = (-1)^i a_{2i}(G)) \quad (1.2)$$

In case G is a forest, then $b_{2i}(G) = m(G, i)$, the number of i -matchings of G .

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*Corresponding author.

Email addresses: shan_haiying@tongji.edu.cn (Hai-Ying Shan), jyshao@tongji.edu.cn (Jia-Yu Shao), lizhang@tongji.edu.cn (Li Zhang), changxianghe@hotmail.com (Chang-Xiang He)

The following integral formula by Gutman and Polansky ([4]) on the difference of the energies of two graphs is the starting point of this paper.

$$\mathbb{E}(G_1) - \mathbb{E}(G_2) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \left| \frac{\phi(G_1, ix)}{\phi(G_2, ix)} \right| dx \quad (i = \sqrt{-1}) \quad (1.3)$$

Now suppose again that G is a bipartite graph of order n . Then by (1.1) and (1.2) we have

$$\phi(G, ix) = i^n \tilde{\phi}(G, x) \quad (G \text{ is bipartite, } i = \sqrt{-1}) \quad (1.4)$$

Using (1.4) we can derive the following new formula from (1.3) which does not involve the complex number i .

Theorem 1.1. *If G_1, G_2 are both bipartite graphs of order n , then we have*

$$\mathbb{E}(G_1) - \mathbb{E}(G_2) = \frac{2}{\pi} \int_0^{+\infty} \ln \frac{\tilde{\phi}(G_1, x)}{\tilde{\phi}(G_2, x)} dx \quad (1.5)$$

Proof. Since G_1, G_2 are both bipartite graphs of order n , it is easy to see that

$$\frac{\tilde{\phi}(G_1, x)}{\tilde{\phi}(G_2, x)} = \frac{\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} b_{2j}(G_1) x^{n-2j}}{\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} b_{2j}(G_2) x^{n-2j}} \text{ is an even function and } \frac{\tilde{\phi}(G_1, x)}{\tilde{\phi}(G_2, x)} > 0 \text{ for } x > 0.$$

So from (1.3) and (1.4) we have

$$\mathbb{E}(G_1) - \mathbb{E}(G_2) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \left| \frac{\phi(G_1, ix)}{\phi(G_2, ix)} \right| dx = \frac{1}{\pi} \int_{-\infty}^{+\infty} \ln \left| \frac{\tilde{\phi}(G_1, x)}{\tilde{\phi}(G_2, x)} \right| dx = \frac{2}{\pi} \int_0^{+\infty} \ln \frac{\tilde{\phi}(G_1, x)}{\tilde{\phi}(G_2, x)} dx.$$

□

Definition 1.1. Let $f(x) = \sum_{i=0}^n a_i x^{n-i}$ and $g(x) = \sum_{i=0}^n b_i x^{n-i}$ be two monic polynomials of degree n with nonnegative coefficients.

- (1). If $a_i \leq b_i$ for all $0 \leq i \leq n$, then we write $f(x) \preceq g(x)$.
- (2). If $f(x) \preceq g(x)$ and $f(x) \neq g(x)$, then we write $f(x) \prec g(x)$.

Now we define the following quasi-order for bipartite graphs (which is equivalent to the well known quasi-order defined by the coefficients $b_i(G)$).

Definition 1.2. Let G_1 and G_2 be two bipartite graphs of order n . Then we write $G_1 \preceq G_2$ if $\tilde{\phi}(G_1, x) \preceq \tilde{\phi}(G_2, x)$, write $G_1 \prec G_2$ if $\tilde{\phi}(G_1, x) \prec \tilde{\phi}(G_2, x)$ and write $G_1 \sim G_2$ if $\tilde{\phi}(G_1, x) = \tilde{\phi}(G_2, x)$.

According to the integral formula in Theorem 1.1, we can see that for two bipartite graphs G_1 and G_2 of order n ,

$$G_1 \preceq G_2 \implies \mathbb{E}(G_1) \leq \mathbb{E}(G_2); \quad \text{and} \quad G_1 \prec G_2 \implies \mathbb{E}(G_1) < \mathbb{E}(G_2).$$

The method of the quasi-order relation “ \preceq ” is an important tool in the study of graph energy.

Graphs with extremal energies are extensively studied in literature. Gutman [1] determined the first and second maximal energy trees of order n ; N.Li, S.Li [8] determined the third maximal energy tree; Gutman et al. [5] conjectured that the fourth maximal energy tree is $P_n(2, 6, n - 9)$ (see Fig.3 for this graph); B. Huo et al. [7] proved that this conjecture is true.

In this paper, we first consider in §2 some recurrence relation of the polynomials $\tilde{\phi}(G(k), x)$ for the k -subdivision graph $G(k)$ (on some cut edge e of a bipartite graph G). Then in §3 we present a new method of directly comparing the energies of two k -subdivision bipartite graphs $G(k)$ and $H(k)$ if they are quasi-order incomparable. Using this new method, we are able to provide a simplified proof of the above mentioned conjecture on the fourth maximal energy tree. The main result of this paper is that, we determine (in §5) the first $\lfloor \frac{n-7}{2} \rfloor$ largest energy trees of order $n \geq 31$ by using the new method of comparing energies given in §3. For example when $n \geq 2007$, we can determine the first 1000 largest energy trees of order n (but up to now, only the first four are known).

2. Some recurrence relations of $\phi(G, x)$ and $\tilde{\phi}(G, x)$ for k -subdivision bipartite graphs

The following lemma is an alternative form of Heilbronner's recurrence formula [6].

Lemma 2.1. [6] *Let uv be a cut edge of a graph G , then $\phi(G, x) = \phi(G - uv, x) - \phi(G - u - v, x)$.*

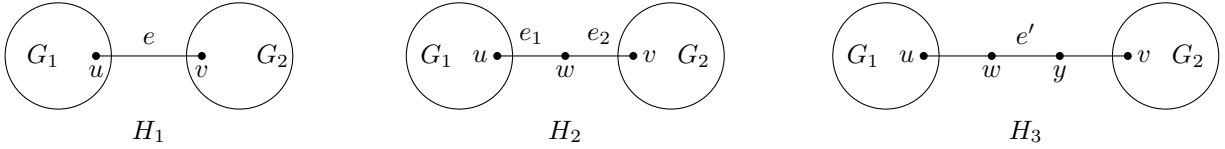


Fig. 1: The graphs H_1, H_2 and H_3

For the sake of simplicity, we sometime abbreviate $\phi(G, x)$ by $\phi(G)$.

The following relation can be derived from Lemma 2.1.

Lemma 2.2. *Let H_1, H_2, H_3 be graphs as shown in Fig.1. Then we have*

$$\phi(H_3, x) = x\phi(H_2, x) - \phi(H_1, x)$$

Proof. Let G'_1 be the graph obtained from G_1 by attaching a new pendent edge uw to G_1 at u , and G'_2 be the graph obtained from G_2 by attaching a new pendent edge vy to G_2 at v . Then by using Lemma 2.1 we have

$$\phi(G'_1) = x\phi(G_1) - \phi(G_1 - u), \quad \text{and} \quad \phi(G'_2) = x\phi(G_2) - \phi(G_2 - v).$$

Now using Lemma 2.1 for H_3 and its cut edge $e' = wy$, we have

$$\begin{aligned} \phi(H_3) &= \phi(H_3 - e') - \phi(H_3 - w - y) = \phi(G'_1)\phi(G'_2) - \phi(G_1)\phi(G_2) \\ &= (x\phi(G_1) - \phi(G_1 - u))(x\phi(G_2) - \phi(G_2 - v)) - \phi(G_1)\phi(G_2) \\ &= (x^2 - 1)\phi(G_1)\phi(G_2) - x\phi(G_1)\phi(G_2 - v) - x\phi(G_2)\phi(G_1 - u) + \phi(G_1 - u)\phi(G_2 - v) \end{aligned}$$

Also using Lemma 2.1 for H_2 and $H_2 - e_1$ we have

$$\begin{aligned} \phi(H_2) &= \phi(H_2 - e_1) - \phi(H_2 - u - w) = \phi(H_2 - e_1 - e_2) - \phi(H_2 - e_1 - w - v) - \phi((G_1 - u) \cup G_2) \\ &= x\phi(G_1)\phi(G_2) - \phi(G_1)\phi(G_2 - v) - \phi(G_1 - u)\phi(G_2) \end{aligned}$$

Using Lemma 2.1 for H_1 we also have

$$\phi(H_1) = \phi(H_1 - e) - \phi(H_1 - u - v) = \phi(G_1)\phi(G_2) - \phi(G_1 - u)\phi(G_2 - v)$$

Now it is easy to verify from the above three equations that $\phi(H_3) = x\phi(H_2) - \phi(H_1)$. □

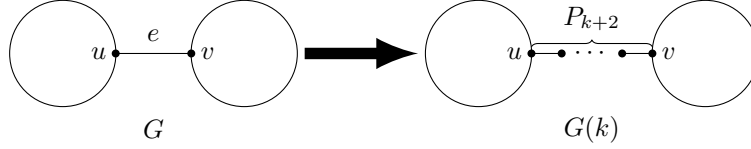


Fig. 2: Graph G and its k -subdivision graph

Definition 2.1. Let e be a cut edge of a graph G , and $G_e(k)$ denote the graph obtained by replacing e with a path of length $k + 1$ (for simplicity of notations, we usually we abbreviate $G_e(k)$ by $G(k)$). We say that $G(k)$ is a k -subdivision graph of G on the cut edge e . We also agree that $G(0) = G$.

From Lemma 2.2, we have the following recurrence relation for $\phi(G(k), x)$.

Theorem 2.1. Let $G(k)$ be a k -subdivision graph of G on the cut edge e of G , then we have

$$\phi(G(k+2), x) = x\phi(G(k+1), x) - \phi(G(k), x) \quad (k \geq 0)$$

Proof. Take $H_1 = G(k)$ in Lemma 2.2 and e be an edge in H_1 on the path of length $k + 1$ obtained by k -subdividing the edge e . Then $H_2 = G(k+1)$ and $H_3 = G(k+2)$. The result now follows from Lemma 2.2. □

Theorem 2.2. Let G be a bipartite graph of order n and $G(k)$ be a k -subdivision graph (of order $n + k$) of G on some cut edge e . Then we have

$$\tilde{\phi}(G(k+2), x) = x\tilde{\phi}(G(k+1), x) + \tilde{\phi}(G(k), x) \quad (k \geq 0) \quad (2.1)$$

Proof. By Theorem 2.1, we have

$$\phi(G(k+2), x) = x\phi(G(k+1), x) - \phi(G(k), x)$$

substitute x by ix , we get

$$\phi(G(k+2), ix) = ix\phi(G(k+1), ix) - \phi(G(k), ix).$$

Now using (1.4) for $G(k+2)$, $G(k+1)$ and $G(k)$ (since they are all bipartite) we have

$$i^{n+k+2}\tilde{\phi}(G(k+2), x) = i^{n+k+1}ix\tilde{\phi}(G(k+1), x) - i^{n+k}\tilde{\phi}(G(k), x)$$

Dividing both sides by i^{n+k+2} we get (2.1). □

Theorem 2.3. Let e, e' be cut edges of bipartite graphs G and H of order n , respectively. If $G(0) \preceq H(0)$ and $G(1) \preceq H(1)$, then we have $G(k) \preceq H(k)$ for all $k \geq 2$, with $G(k) \sim H(k)$ if and only if both the two relations $H(0) \sim G(0)$ and $H(1) \sim G(1)$ hold.

Proof. The result follows directly from Theorem 2.2 and induction on k . \square

Theorem 2.4. Let G, H be bipartite graphs of order n , e_1, e_2 be two cut edges of G and e'_1, e'_2 be two cut edges of H . Let $G(a, b)$ denote the graph obtained from G by subdividing e_1, e_2 by a, b times, and $H(c, d)$ denote the graph obtained from H by subdividing e'_1, e'_2 by c, d times, respectively. If

$$G(0, 0) \preceq H(0, 0) \quad \text{and} \quad G(0, 1) \preceq H(0, 1), \quad (2.2)$$

$$G(1, 0) \preceq H(1, 0) \quad \text{and} \quad G(1, 1) \preceq H(1, 1) \quad (2.3)$$

then we have $G(l, k) \preceq H(l, k)$ for all $l \geq 0$ and $k \geq 0$. Moreover, if one of l and k is at least 2, then $G(l, k) \prec H(l, k)$ if each of (2.2) and (2.3) contains at least one strict relation.

Proof. Using Theorem 2.3 for e_2 and e'_2 we have

$$(2.2) \implies G(0, k) \preceq H(0, k) \quad (k \geq 0), \quad (2.4)$$

$$(2.3) \implies G(1, k) \preceq H(1, k) \quad (k \geq 0). \quad (2.5)$$

Now using Theorem 2.3 for e_1 and e'_1 we also have

$$(2.4) \text{ and } (2.5) \implies G(l, k) \preceq H(l, k) \quad (l \geq 0).$$

When (2.2) and (2.3) both contain strict relations, we have both strict relations in (2.4) and (2.5) for $k \geq 2$. Thus $G(l, k) \prec H(l, k)$ for all $k \geq 2$ by Theorem 2.3. Similar arguments apply to the case $l \geq 2$. \square

3. A new method of directly comparing the energies of k -subdivision bipartite graphs

Notice that if the conditions in Theorem 2.3 do not hold, then $G(k)$ and $H(k)$ might be quasi-order incomparable. In this section, we present a new method to directly compare the energies of two k -subdivision bipartite graphs $G(k)$ and $H(k)$ when they are quasi-order incomparable. Using this method, we give a simplified proof of the conjecture on the fourth maximal energy tree.

In the following, we always write $g_k = \tilde{\phi}(G(k), x)$, $h_k = \tilde{\phi}(H(k), x)$, and $d_k = \frac{h_k}{g_k}$.

Lemma 3.1. Let $G(k), H(k)$ be k -subdivision graphs on some cut edges of the bipartite graphs G and H of order n , respectively ($k \geq 0$), g_k, h_k and d_k be defined as above. Then for each fixed $x > 0$, we have

(1). If $d_1 > d_0$, then $d_0 < d_k < d_1$ for all $k \geq 2$;

(2). If $d_1 < d_0$, then $d_1 < d_k < d_0$ for all $k \geq 2$;

(3). If $d_1 = d_0$, then $d_k = d_0$ for all k .

(So in any case we have $d_k \geq \min\{d_0, d_1\}$.)

Proof. By the recurrence relations in Theorem 2.2, we have

$$\begin{aligned} d_k &= \frac{h_k}{g_k} = \frac{xh_{k-1} + h_{k-2}}{xg_{k-1} + g_{k-2}} = \frac{xd_{k-1}g_{k-1} + d_{k-2}g_{k-2}}{xg_{k-1} + g_{k-2}} \\ &= \left(\frac{xg_{k-1}}{xg_{k-1} + g_{k-2}} \right) d_{k-1} + \left(\frac{g_{k-2}}{xg_{k-1} + g_{k-2}} \right) d_{k-2} \end{aligned}$$

This tells us that d_k is a convex combination of d_{k-1} and d_{k-2} with positive coefficients, which implies that d_k lies in the open interval (d_{k-1}, d_{k-2}) or (d_{k-2}, d_{k-1}) if $d_{k-1} \neq d_{k-2}$. Using this fact and the induction on k we obtain that d_k always lies in the open interval (d_0, d_1) or (d_1, d_0) when $d_0 \neq d_1$, and $d_k = d_0$ when $d_1 = d_0$. \square

The following theorem can be derived from Lemma 3.1:

Theorem 3.1. (1). If $h_1g_0 - h_0g_1 = \tilde{\phi}(H(1), x)\tilde{\phi}(G(0), x) - \tilde{\phi}(H(0), x)\tilde{\phi}(G(1), x) > 0$ (which is equivalent to $d_1(x) > d_0(x)$) for all $x > 0$, then we have

$$\mathbb{E}(H(k)) - \mathbb{E}(G(k)) > \mathbb{E}(H(0)) - \mathbb{E}(G(0)) \quad (\text{for all } k > 0.)$$

(2). If $h_1g_0 - h_0g_1 = \tilde{\phi}(H(1), x)\tilde{\phi}(G(0), x) - \tilde{\phi}(H(0), x)\tilde{\phi}(G(1), x) < 0$ (which is equivalent to $d_1(x) < d_0(x)$) for all $x > 0$, then we have

$$\mathbb{E}(H(k)) - \mathbb{E}(G(k)) > \mathbb{E}(H(1)) - \mathbb{E}(G(1)) \quad \text{for all } k \neq 1.$$

Proof. (1). Since $d_1(x) > d_0(x)$ for all $x > 0$, by (1) of Lemma 3.1 we have $d_k(x) > d_0(x)$ for all $x > 0$ and $k > 0$. So by (1.5) we have

$$\begin{aligned} \mathbb{E}(H(k)) - \mathbb{E}(G(k)) &= \frac{2}{\pi} \int_0^{+\infty} \ln \frac{\tilde{\phi}(H(k), x)}{\tilde{\phi}(G(k), x)} dx = \frac{2}{\pi} \int_0^{+\infty} \ln d_k(x) dx \\ &> \frac{2}{\pi} \int_0^{+\infty} \ln d_0(x) dx = \frac{2}{\pi} \int_0^{+\infty} \ln \frac{\tilde{\phi}(H(0), x)}{\tilde{\phi}(G(0), x)} dx = \mathbb{E}(H(0)) - \mathbb{E}(G(0)) \quad (k > 0). \end{aligned}$$

The proof of (2) is similar to that of (1). \square

In [9], Shan et al. show that the fourth largest energy tree is either $P_n(2, 6, n-9)$ or $T_n(2, 2|2, 2)$ (see Fig.3 and Fig.4 for the definitions of these two graphs). B. Huo et al.[7] proved that the conjecture on the fourth maximal energy tree is true by showing that $\mathbb{E}(P_n(2, 6, n-9)) > \mathbb{E}(T_n(2, 2|2, 2))$. Now by using Theorem 3.1, we are able to give a simplified proof of the conjecture on the fourth maximal energy tree.

Theorem 3.2. If $n \geq 10$, then

$$\mathbb{E}(P_n(2, 6, n-9)) > \mathbb{E}(T_n(2, 2|2, 2))$$

Proof. Let $H = P_{10}(2, 6, 1)$ and $G = T_{10}(2, 2|2, 2)$, e be the pendent edge on the pendent path of length 1 in H , and e' be the edge between the two vertices of degree 3 in G . Then we have $P_n(2, 6, n-9) = H(n-10)$ and $T_n(2, 2|2, 2) = G(n-10)$. By some directly calculations, we have

$$\begin{aligned} \tilde{\phi}(H(0), x) &= \tilde{\phi}(P_{10}(2, 6, 1), x) = x^{10} + 9x^8 + 27x^6 + 31x^4 + 12x^2 + 1, \\ \tilde{\phi}(G(0), x) &= \tilde{\phi}(T_{10}(2, 2|2, 2), x) = x^{10} + 9x^8 + 26x^6 + 30x^4 + 13x^2 + 1, \\ \tilde{\phi}(H(1), x) &= \tilde{\phi}(P_{11}(2, 6, 2), x) = x^{11} + 10x^9 + 35x^7 + 52x^5 + 32x^3 + 6x, \\ \tilde{\phi}(G(1), x) &= \tilde{\phi}(T_{11}(2, 2|2, 2), x) = x^{11} + 10x^9 + 34x^7 + 48x^5 + 29x^3 + 6x. \end{aligned}$$

So we have

$$\tilde{\phi}(H(1), x)\tilde{\phi}(G(0), x) - \tilde{\phi}(H(0), x)\tilde{\phi}(G(1), x) = 2x^{15} + 22x^{13} + 89x^{11} + 168x^9 + 156x^7 + 66x^5 + 9x^3 > 0 \quad (x > 0).$$

Also by using computer we can obtain

$$\mathbb{E}(H(0)) \doteq 11.937511, \quad \mathbb{E}(G(0)) \doteq 11.924777, \quad \text{So } \mathbb{E}(H(0)) - \mathbb{E}(G(0)) \doteq 0.012734 > 0.$$

So by Theorem 3.1 we have for $n \geq 10$,

$$\mathbb{E}(P_n(2, 6, n-9)) - \mathbb{E}(T_n(2, 2|2, 2)) = \mathbb{E}(H(n-10)) - \mathbb{E}(G(n-10)) \geq \mathbb{E}(H(0)) - \mathbb{E}(G(0)) > 0. \quad \square$$

Combining Theorem 3.2 with the result that the fourth largest energy tree is either $P_n(2, 6, n-9)$ or $T_n(2, 2|2, 2)$ ([9]), we conclude that the fourth maximal energy tree is $P_n(2, 6, n-9)$.

Remark: Here we would like to mention that, the main points of the simplification in the proof of Theorem 3.2 are:

1. We use the integral formula (1.5) (instead of (1.3)) which uses the real polynomial $\tilde{\phi}(G_j, x)$ instead of the complex polynomial $\phi(G_j, ix)$ for $j = 1, 2$.

2. The recurrence relation (2.1) for $\tilde{\phi}(G(k), x)$ allows us to use Lemma 3.1 to directly compare $d_k(x)$ and $d_0(x)$ (namely directly compare the integrands $\ln d_k(x)$ and $\ln d_0(x)$ in the formula (1.5) for $\mathbb{E}(H(k)) - \mathbb{E}(G(k))$ and $\mathbb{E}(H(0)) - \mathbb{E}(G(0))$), without the need of solving the recurrence relation (2.1) to obtain explicit expressions for $h_k = \tilde{\phi}(H(k), x)$ and $g_k = \tilde{\phi}(G(k), x)$. \square

Notice that in Theorem 3.1, we need either $d_1(x) > d_0(x)$ for all $x > 0$ or $d_0(x) > d_1(x)$ for all $x > 0$. Now if both of these two conditions do not hold, then both $d_0(x)$ and $d_1(x)$ are not a lower bound for $d_k(x)$ ($k \geq 2$). Although in this case we can not use Theorem 3.1, but by Lemma 3.1 we still have $\min\{d_0(x), d_1(x)\}$ as a lower bound for $d_k(x)$ (for all $x > 0$). Thus we can still have the following lower bound (which is independent of k) for $\mathbb{E}(H(k)) - \mathbb{E}(G(k))$.

Theorem 3.3. *Let $G(k)$, $H(k)$ be k -subdivision graphs of bipartite graphs G and H on some cut edges. Let $d_k(x) = \frac{\tilde{\phi}(H(k), x)}{\tilde{\phi}(G(k), x)}$ and let $D = \{x > 0 | d_0(x) > d_1(x)\}$, Let D^C be the complement of D in $(0, \infty)$. Then :*

$$\mathbb{E}(H(k)) - \mathbb{E}(G(k)) \geq \frac{2}{\pi} \int_0^{+\infty} \ln \min\{d_0(x), d_1(x)\} dx = \frac{2}{\pi} \int_D \ln d_1(x) dx + \frac{2}{\pi} \int_{D^C} \ln d_0(x) dx \quad (3.1)$$

where the right hand side of (3.1) can also be written as:

$$\begin{aligned} \frac{2}{\pi} \int_D \ln d_1(x) dx + \frac{2}{\pi} \int_{D^C} \ln d_0(x) dx &= \frac{2}{\pi} \int_0^{+\infty} \ln d_1(x) dx - \frac{2}{\pi} \int_{D^C} \ln d_1(x) dx + \frac{2}{\pi} \int_{D^C} \ln d_0(x) dx \\ &= \mathbb{E}(H(1)) - \mathbb{E}(G(1)) - \frac{2}{\pi} \int_{D^C} \ln \frac{d_1(x)}{d_0(x)} dx \end{aligned} \quad (3.2)$$

or equivalently,

$$\frac{2}{\pi} \int_D \ln d_1(x) dx + \frac{2}{\pi} \int_{D^C} \ln d_0(x) dx = \mathbb{E}(H(0)) - \mathbb{E}(G(0)) + \frac{2}{\pi} \int_D \ln \frac{d_1(x)}{d_0(x)} dx \quad (3.3)$$

Theorem 3.3 will be used several times in §4 and §5 in the proof of our main results.

4. Some upper bounds for the energies of non-starlike trees

In the following discussions, we will divide the trees into two classes. One is called the starlike trees, and the other one is the non-starlike trees. In this section, We will give some upper bounds for the energies of

the non-starlike trees. We will show that the energy of a non-starlike tree is bounded above either by the energy of $P_n(1, 2, n-4)$, or by the energy of $T_n(2, 2|2, 2)$ (see Fig.3 and Fig.4).

Let $N_3(G)$ be the number of vertices in G with degree at least 3, and $\Delta(G)$ be the maximal degree of G . A tree T is called starlike if $N_3(T) \leq 1$, and is called non-starlike if $N_3(T) \geq 2$.

It is easy to see that if $N_3(T) = 0$, then T is the path P_n . Now if $N_3(T) = 1$, then T consists of some internally disjoint pendent paths starting from its unique vertex with degree at least 3. Suppose that the lengths of these pendent paths are positive integers a_1, a_2, \dots, a_k . Then we denote this tree T by $P_n(a_1, a_2, \dots, a_k)$, where $a_1 + a_2 + \dots + a_k = n-1$ and $k = \Delta(T)$ (see Fig.3). Sometimes we also denote $P_n(a_1, a_2, \dots, a_k)$ by $P_n(a_1, a_2, \dots, a_{k-1}, *)$, since $*$ is uniquely determined by n and a_1, a_2, \dots, a_{k-1} .

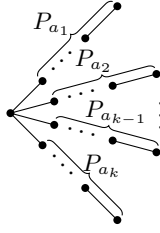


Fig. 3: The starlike tree $P_n(a_1, a_2, \dots, a_k)$

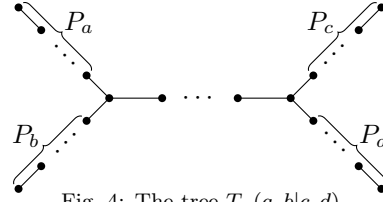


Fig. 4: The tree $T_n(a, b|c, d)$

Let a, b, c, d be positive integers with $a + b + c + d \leq n-2$. Let $T_n(a, b|c, d)$ be the tree of order n obtained by attaching two pendent paths of lengths a and b to one end vertex of the path $P_{n-a-b-c-d}$, and attaching two pendent paths of lengths c and d to another end vertex of the path $P_{n-a-b-c-d}$ (see Fig.4).

It is not difficult to see that if T is a tree of order n with $\Delta(T) = 3$ and $N_3(T) = 2$, then T must be of the form $T_n(a, b|c, d)$, where $a + b + c + d \leq n-2$.

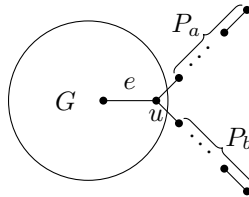


Fig. 5: The graph $G_u(a, b)$

In [9] and [10], Shan et al. studied how graph energies change under edge grafting operations on unicyclic or bipartite graphs and proved the following result in the comparison of the quasi-order on unicyclic or bipartite graphs:

Lemma 4.1. ([9], The edge grafting operation) *Let u be a vertex of a graph G . Denote $G_u(a, b)$ the graph obtained by attaching to G two (new) pendent paths of lengths a and b at u . Let a, b, c, d be nonnegative integers with $a + b = c + d$. Assume that $0 \leq a \leq b$, $0 \leq c \leq d$ and $a < c$. If u is a non-isolated vertex of a unicyclic or bipartite graph G , then the following statements are true:*

- (1). *If a is even, then $G_u(a, b) \succ G_u(c, d)$.*
- (2). *If a is odd, then $G_u(a, b) \prec G_u(c, d)$.*

If $a = 0$, then we say that $G_u(0, b)$ is obtained from $G_u(c, d)$ by a *total edge grafting* operation.

The following result in [9] was obtained directly by using the edge grafting operation.

Theorem 4.1. [9] Let T be a tree of order n with $N_3(T) \geq 2$. Then there exists a tree T' of order n with $N_3(T') = N_3(T) - 1$ and $\Delta(T') = \Delta(T)$ such that $T \prec T'$.

In the followings, we will give some upper bounds for the energies of the trees of the form $T_n(a, b|c, d)$. First we consider the case $1 \in \{a, b, c, d\}$ in the following Theorem 4.2. The other case where $\min\{a, b, c, d\} \geq 2$ will be considered in Lemma 4.3, 4.4 and Theorem 4.3.

Theorem 4.2. [9] Let $T = T_n(1, b|c, d)$. Then $T \prec P_n(1, 2, n - 4)$.

Proof. By using total edge grafting on the two pendent paths of lengths c and d , we have $T \prec P_n(1, b, n - 2 - b)$. Using the edge grafting operation again, we have $P_n(1, b, n - 2 - b) \preceq P_n(1, 2, n - 4)$. Thus the result follows. \square

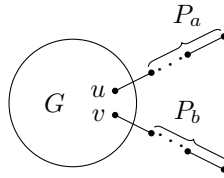


Fig. 6: $G_{u,v}(a, b)$

The following Lemma generalizes Lemma 4.1, and is called “edge grafting operation at different vertices”.

Lemma 4.2. [10] Let u, v be two vertices of a unicyclic or bipartite graph G . Let $G_{u,v}(a, b)$ be the graph obtained from G by attaching a pendent path of length a to u and attaching a pendent path of length b to v (as shown in Fig.6). Suppose that G satisfies:

- (i). $G_{u,v}(0, 2) \succ G_{u,v}(1, 1)$.
- (ii). For any nonnegative integers p, q , $G_{u,v}(p, q) = G_{u,v}(q, p)$.

Let a, b, c, d be nonnegative integers with $a \leq b$, $c \leq d$, $a + b = c + d$, and $a < c$, then we have

- (1) If a is even, then $G_{u,v}(a, b) \succ G_{u,v}(c, d)$.
- (2) If a is odd, then $G_{u,v}(a, b) \prec G_{u,v}(c, d)$.



Fig. 7: $T_{12}(3, 2|2, 2)$ and $T_{12}(2, 2|2, 2)$

Now we use the methods given in §3 to prove the following two lemmas, which consider the tree $T_n(a, 2|2, 2)$ in two cases $3 \leq a \leq n - 9$ and $a = n - 8$. These two lemmas will only be used in the proof of the Theorem 4.3 later.

Lemma 4.3. Let $3 \leq a \leq n - 9$. Then $T_n(a, 2|2, 2) \prec T_n(2, 2|2, 2)$.

Proof. Let e_1, e_2 be the cut edges of $G = T_{12}(3, 2|2, 2)$ and e'_1, e'_2 be the cut edges of $H = T_{12}(2, 2|2, 2)$ as shown in Fig.7. respectively. Then we have $T_n(a, 2|2, 2) = G(a - 3, n - 9 - a)$ and $T_n(2, 2|2, 2) = H(a - 3, n - 9 - a)$.

By some directly calculations, we have

$$\begin{aligned}
\tilde{\phi}(H(0,0),x) &= \tilde{\phi}(T_{12}(2,2|2,2),x) = x^{12} + 11x^{10} + 43x^8 + 74x^6 + 59x^4 + 19x^2 + 1, \\
\tilde{\phi}(G(0,0),x) &= \tilde{\phi}(T_{12}(3,2|2,2),x) = x^{12} + 11x^{10} + 43x^8 + 74x^6 + 57x^4 + 17x^2, \\
\tilde{\phi}(H(1,0),x) &= \tilde{\phi}(H(0,1),x) = \tilde{\phi}(T_{13}(2,2|2,2),x) = x^{13} + 12x^{11} + 53x^9 + 108x^7 + 107x^5 + 48x^3 + 7x, \\
\tilde{\phi}(G(1,0),x) &= \tilde{\phi}(T_{13}(4,2|2,2),x) = x^{13} + 12x^{11} + 53x^9 + 108x^7 + 105x^5 + 46x^3 + 7x, \\
\tilde{\phi}(G(0,1),x) &= \tilde{\phi}(T_{13}(3,2|2,2),x) = x^{13} + 12x^{11} + 53x^9 + 108x^7 + 106x^5 + 46x^3 + 6x, \\
\tilde{\phi}(H(1,1),x) &= \tilde{\phi}(T_{14}(2,2|2,2),x) = x^{14} + 13x^{12} + 64x^{10} + 151x^8 + 181x^6 + 107x^4 + 26x^2 + 1, \\
\tilde{\phi}(G(1,1),x) &= \tilde{\phi}(T_{14}(4,2|2,2),x) = x^{14} + 13x^{12} + 64x^{10} + 151x^8 + 180x^6 + 105x^4 + 25x^2 + 1.
\end{aligned}$$

By comparing the coefficients of above polynomials, we find that

$$G(0,0) \prec H(0,0), \quad G(0,1) \prec H(0,1), \quad G(1,0) \prec H(1,0), \quad G(1,1) \prec H(1,1).$$

So by Theorem 2.4 we have $T_n(a, 2|2, 2) = G(a-3, n-9-a) \prec H(a-3, n-9-a) = T_n(2, 2|2, 2)$. \square

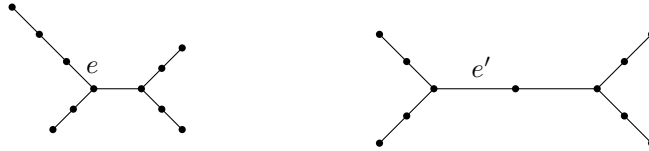


Fig. 8: $G = T_{11}(3, 2|2, 2)$ and $H = T_{11}(2, 2|2, 2)$

Now we consider the remaining case $a = n - 8$ for the trees of the form $T_n(a, 2|2, 2)$.

Lemma 4.4. $\mathbb{E}(T_n(n-8, 2|2, 2)) < \mathbb{E}(T_n(2, 2|2, 2))$ for all $n \geq 11$.

Proof. Consider the cut edges e of $G = T_{11}(3, 2|2, 2)$ and e' of $H = T_{11}(2, 2|2, 2)$ as shown in Fig.8. Let $G(k)$, $H(k)$ be graphs obtained by subdividing the cut edges e of G and e' of H respectively k times. Then we have $T_n(n-8, 2|2, 2) = G(n-11)$ and $T_n(2, 2, 2, 2) = H(n-11)$. Denote $g_k = \tilde{\phi}(G(k), x)$ and $h_k = \tilde{\phi}(H(k), x)$.

By some directly calculations, we have

$$\begin{aligned}
h_0 &= \tilde{\phi}(T_{11}(2, 2|2, 2), x) = x^{11} + 10x^9 + 34x^7 + 48x^5 + 29x^3 + 6x, \\
g_0 &= \tilde{\phi}(T_{11}(3, 2|2, 2), x) = x^{11} + 10x^9 + 34x^7 + 49x^5 + 29x^3 + 5x, \\
h_1 &= \tilde{\phi}(T_{12}(2, 2|2, 2), x) = x^{12} + 11x^{10} + 43x^8 + 74x^6 + 59x^4 + 19x^2 + 1, \\
g_1 &= \tilde{\phi}(T_{12}(4, 2|2, 2), x) = x^{12} + 11x^{10} + 43x^8 + 75x^6 + 59x^4 + 18x^2 + 1.
\end{aligned}$$

So we have

$$h_1g_0 - h_0g_1 = x(x-1)(x+1)(x^6 + 7x^4 + 11x^2 + 1)(x^2 + 1)^3.$$

Thus

$$D = \{x | h_1g_0 - h_0g_1 < 0, x > 0\} = (0, 1).$$

Also by using computer we can find:

$$\mathbb{E}(H(0)) \doteq 13.059967, \quad \mathbb{E}(G(0)) \doteq 13.015698$$

and by using computer to calculate the integral we can further obtain

$$\mathbb{E}(H(0)) - \mathbb{E}(G(0)) + \frac{2}{\pi} \int_D \ln \frac{d_1(x)}{d_0(x)} dx = \mathbb{E}(H) - \mathbb{E}(G) + \frac{2}{\pi} \int_0^1 \ln \frac{h_1 g_0}{h_0 g_1} dx \doteq 0.005951 > 0.$$

So using Theorem 3.3, we obtain $\mathbb{E}(H(k)) - \mathbb{E}(G(k)) > 0$ for all $k \geq 0$. Thus $\mathbb{E}(T_n(n-8, 2|2, 2)) < \mathbb{E}(T_n(2, 2|2, 2))$. \square

Theorem 4.3. *Let $n \geq 11$, $a, b, c, d \geq 2$ and a, b, c, d are not all equal to 2. Then we have*

$$\mathbb{E}(T_n(a, b|c, d)) < \mathbb{E}(T_n(2, 2|2, 2)).$$

Proof. By using the edge grafting operation in Lemma 4.1, we have

$$T_n(a, b|c, d) \preceq T_n(a+b-2, 2|2, c+d-2).$$

By using Lemma 4.2 (edge grafting on different vertices), we also have

$$T_n(a+b-2, 2|2, c+d-2) \preceq T_n(a+b+c+d-6, 2|2, 2).$$

Write $x = a+b+c+d-6$, then we have $3 \leq x \leq n-8$ since at least one of a, b, c, d is greater than 2.

Now If $3 \leq x \leq n-9$, then by Lemma 4.3 we have $T_n(x, 2|2, 2) \prec T_n(2, 2|2, 2)$. So $\mathbb{E}(T_n(a, b|c, d)) \leq \mathbb{E}(T_n(x, 2|2, 2)) < \mathbb{E}(T_n(2, 2|2, 2))$.

If $x = n-8$, then by Lemma 4.4 we have $\mathbb{E}(T_n(a, b|c, d)) \leq \mathbb{E}(T_n(x, 2|2, 2)) < \mathbb{E}(T_n(2, 2|2, 2))$. \square

5. The trees of order n with the first $\lfloor \frac{n-7}{2} \rfloor$ largest energies

In this section, we will determine the first $\lfloor \frac{n-7}{2} \rfloor$ largest energy trees of order $n \geq 31$ by using the method of directly comparing energies given in §3.

First, we divide the class of starlike trees into the following four subclasses:

(C1). The path P_n .

(C2). The class $S_n = \{P_n(2, a, b) \mid a+b = n-3, 1 \leq a \leq b\}$.

(C3). The starlike trees T of order n with $\Delta(T) = 3$ and $T \notin S_n$.

(C4). The starlike trees T of order n with $\Delta(T) \geq 4$.

For convenience, we also define the following class (C5):

(C5). The class of non-starlike trees of order n (i.e., $N_3(T) \geq 2$).

It is obvious that the union of the classes (C1)-(C5) is the class of all the trees of order n .

Now, our strategy of proving the main result is as follows. Firstly, using the quasi-order we can obtain (in Theorem 5.1) a total ordering of all the $\lfloor \frac{n-3}{2} \rfloor$ trees in S_n . Secondly, we can show (in Theorem 5.2) that the maximal tree (under the quasi-order) in the class (C3) is $P_n(4, 4, *)$, and the maximal tree in the class (C4) is $P_n(2, 2, 2, *)$. Next, by directly comparing the energies of the largest energy trees in the classes (C3) and (C4) with some smaller energy graphs in S_n , and comparing the energies of the tree $T_n(2, 2|2, 2)$ in the class (C5) with the smallest energy tree $P_n(2, 1, n-4)$ in S_n , we obtain that the first $\lfloor \frac{n-9}{2} \rfloor$ largest energy trees in S_n together with P_n are the first $\lfloor \frac{n-7}{2} \rfloor$ largest energy trees in the class of all trees of order n .

Theorem 5.1. Let $S_n = \{P_n(2, a, b) \mid a + b = n - 3, 1 \leq a \leq b\}$. Let $k = \lfloor \frac{n-3}{2} \rfloor$, $t = \lfloor \frac{k}{2} \rfloor$ and $l = \lfloor \frac{k-1}{2} \rfloor$. Then we have the following totally quasi order for the trees in S_n :

$$P_n(2, 2, *) \succ P_n(2, 4, *) \succ \cdots \succ P_n(2, 2t, *) \succ P_n(2, 2l + 1, *) \succ \cdots \succ P_n(2, 3, *) \succ P_n(2, 1, *). \quad (5.1)$$

Proof. The result follows directly from Lemma 4.1 by using the edge grafting operation. \square

Theorem 5.2. Let $n \geq 11$. Then we have

- (1). If $T \in (C3)$ and $T \neq P_n(4, 4, n - 9)$, then $T \prec P_n(4, 4, n - 9)$.
- (2). If $T \in (C4)$ and $T \neq P_n(2, 2, 2, n - 7)$, then $T \prec P_n(2, 2, 2, n - 7)$.

Proof. (1) Since $T \in (C3)$, T must be of the form $P_n(a, b, c)$ with $2 \notin \{a, b, c\}$. Without loss of generality, we may assume that $a \leq b \leq c$. Then $b + c \geq 7$ since $n \geq 11$. So by Lemma 4.1 we have $T = P_n(a, b, c) \preceq P_n(a, 4, b + c - 4)$ and $P_n(a, 4, b + c - 4) \preceq P_n(4, 4, n - 9)$ since $b + c - 4 \neq 2$. Also $T \neq P_n(4, 4, n - 9)$ implies at least one of the above two relations is strict. Thus we have $T = P_n(a, b, c) \prec P_n(4, 4, n - 9)$.

(2) Since $\Delta(T) \geq 4$ for $T \in (C4)$, by using Lemma 4.1 we can derive that $T \preceq P_n(a, b, c, d)$ for some tree $P_n(a, b, c, d)$. By further using the edge grafting operations at most 3 times on $P_n(a, b, c, d)$, we will finally obtain $P_n(a, b, c, d) \preceq P_n(2, 2, 2, n - 7)$. Also $T \neq P_n(2, 2, 2, n - 7)$ implies at least one of the above relations is strict. Thus we have $T \prec P_n(2, 2, 2, n - 7)$. \square

The following Theorem 5.3 and Theorem 5.4 will exclude out $P_n(2, 2, 2, *)$ (the maximal energy tree in the class (C4)) and $T_n(2, 2|2, 2)$ (in (C5)) by the smallest energy tree in S_n by using the method of directly comparing energies given in §3.



Fig. 9: $P_9(2, 2, 2, 2)$ and $P_9(2, 1, 5)$

Theorem 5.3. Let $n \geq 10$. Then we have $\mathbb{E}(P_n(2, 2, 2, n - 7)) < \mathbb{E}(P_n(2, 1, n - 4))$

Proof. Consider the cut edges e of $G = P_9(2, 2, 2, 2)$ and e' of $H = P_9(2, 1, 5)$ as shown in Fig.9.

Let $G(k)$, $H(k)$ be graphs obtained by subdividing the cut edges e of G and e' of H respectively k times. Then we have $P_n(2, 2, 2, n - 7) = G(n - 9)$ and $P_n(2, 1, n - 4) = H(n - 9)$. Denote $g_k = \tilde{\phi}(G(k), x)$ and $h_k = \tilde{\phi}(H(k), x)$.

By some directly calculations, we have

$$\begin{aligned} h_0 &= \tilde{\phi}(P_9(2, 1, 5), x) = x^9 + 8x^7 + 20x^5 + 17x^3 + 4x, \\ g_0 &= \tilde{\phi}(P_9(2, 2, 2, 2), x) = x^9 + 8x^7 + 18x^5 + 16x^3 + 5x, \\ h_1 &= \tilde{\phi}(P_{10}(2, 1, 6), x) = x^{10} + 9x^8 + 27x^6 + 31x^4 + 12x^2 + 1, \\ g_1 &= \tilde{\phi}(P_{10}(2, 2, 2, 3), x) = x^{10} + 9x^8 + 25x^6 + 28x^4 + 12x^2 + 1. \end{aligned}$$

So we have $h_1g_0 - h_0g_1 = (2x^4 + 8x^2 + 1)(x^2 + 1)^3 > 0$ for all $x > 0$.

Also we can compute that $\mathbb{E}(H(0)) = \mathbb{E}(G(0)) = 6 + 2\sqrt{5}$. So using Theorem 3.1, we have

$$\mathbb{E}(P_n(2, 1, n - 4)) - \mathbb{E}(P_n(2, 2, 2, n - 7)) = \mathbb{E}(H(n - 9)) - \mathbb{E}(G(n - 9)) > \mathbb{E}(H(0)) - \mathbb{E}(G(0)) = 0. \quad \square$$

Notice that $P_n(2, 2, 2, n-7)$ and $P_n(2, 1, n-4)$ are quasi-order incomparable when $n \geq 11$. So Theorem 5.3 can not be proven by only using the quasi-order method.

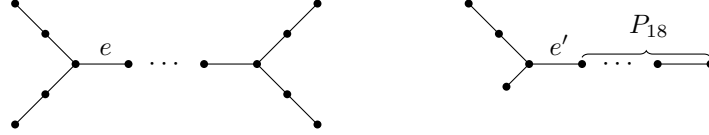


Fig. 10: $T_{22}(2, 2|2, 2)$ and $P_{22}(2, 1, 18)$

Theorem 5.4. *Let $n \geq 22$. Then we have $\mathbb{E}(T_n(2, 2|2, 2)) < \mathbb{E}(P_n(2, 1, n-4))$.*

Proof. Consider the cut edges e of $G = T_{22}(2, 2|2, 2)$ and e' of $H = P_{22}(2, 1, 18)$ as shown in Fig.10.

Let $G(k), H(k)$ be graphs obtained by subdividing the cut edges e of G and e' of H respectively k times. Then we have $T_n(2, 2|2, 2) = G(n-22)$ and $P_n(2, 1, n-4) = H(n-22)$. Denote $g_k = \tilde{\phi}(G(k), x)$ and $h_k = \tilde{\phi}(H(k), x)$.

By some directly calculations, we have

$$\begin{aligned} h_0 &= x^{22} + 21x^{20} + 189x^{18} + 953x^{16} + 2955x^{14} + 5824x^{12} + 7293x^{10} + 5643x^8 + 2541x^6 + 595x^4 + 57x^2 + 1, \\ g_0 &= x^{22} + 21x^{20} + 188x^{18} + 939x^{16} + 2879x^{14} + 5625x^{12} + 7046x^{10} + 5546x^8 + 2598x^6 + 644x^4 + 64x^2 + 1, \\ h_1 &= x^{23} + 22x^{21} + 209x^{19} + 1123x^{17} + 3756x^{15} + 8113x^{13} + 11375x^{11} + 10153x^9 + 5511x^7 + 1672x^5 \\ &\quad + 241x^3 + 11x, \\ g_1 &= x^{23} + 22x^{21} + 208x^{19} + 1108x^{17} + 3667x^{15} + 7850x^{13} + 10982x^{11} + 9912x^9 + 5546x^7 + 1768x^5 \\ &\quad + 268x^3 + 12x. \end{aligned}$$

So we have

$$h_1g_0 - h_0g_1 = x(x^8 + 7x^6 + 11x^4 - 4x^2 - 1)(x^2 + 1)^3$$

$$D = \{x | h_1g_0 - h_0g_1 < 0, x > 0\} \doteq (0, 0.663073).$$

By using computer we can also find

$$\mathbb{E}(H(0)) \doteq 27.182092, \quad \mathbb{E}(G(0)) \doteq 27.175139, \quad \text{and} \quad \mathbb{E}(H(0)) - \mathbb{E}(G(0)) + \frac{2}{\pi} \int_D \ln\left(\frac{h_1g_0}{h_0g_1}\right) dx \doteq 0.000425 > 0.$$

So by using Theorem 3.3, we have $\mathbb{E}(P_n(2, 1, n-4)) - \mathbb{E}(T_n(2, 2|2, 2)) = \mathbb{E}(H(n-22)) - \mathbb{E}(G(n-22)) > 0$. \square

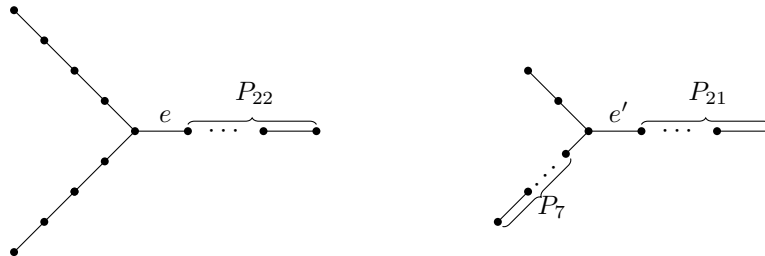


Fig. 11: $P_{31}(4, 4, 22)$ and $P_{31}(2, 7, 21)$

The following Theorem 5.5 will exclude out the maximal energy tree in the class (C3) by the fourth smallest energy tree in S_n .

Theorem 5.5. *Let $n \geq 31$. Then we have $\mathbb{E}(P_n(4, 4, n - 9)) < \mathbb{E}(P_n(2, 7, n - 10))$.*

Proof. Consider the cut edges e of $G = P_{31}(4, 4, 22)$ and e' of $H = P_{31}(2, 7, 21)$ as shown in Fig.11.

Let $G(k)$, $H(k)$ be graphs obtained by subdividing the cut edges e of G and e' of H respectively k times. Then we have $P_n(4, 4, n - 9) = G(n - 31)$ and $P_n(2, 7, n - 10) = H(n - 31)$. Denote $g_k = \tilde{\phi}(G(k), x)$ and $h_k = \tilde{\phi}(H(k), x)$.

By some directly calculations, we have

$$\begin{aligned} h_0 &= \tilde{\phi}(P_{31}(2, 7, 21), x) = x^{31} + 30x^{29} + 405x^{27} + 3252x^{25} + 17296x^{23} + 64220x^{21} + 170943x^{19} + 329768x^{17} \\ &\quad + 460696x^{15} + 460851x^{13} + 322620x^{11} + 152131x^9 + 45426x^7 + 7738x^5 + 619x^3 + 15x, \\ g_0 &= \tilde{\phi}(P_{31}(4, 4, 22), x) = x^{31} + 30x^{29} + 405x^{27} + 3252x^{25} + 17295x^{23} + 64200x^{21} + 170772x^{19} + 328952x^{17} \\ &\quad + 458317x^{15} + 456496x^{13} + 317681x^{11} + 148864x^9 + 44349x^7 + 7644x^5 + 636x^3 + 16x, \\ h_1 &= \tilde{\phi}(P_{32}(2, 7, 22), x) = x^{32} + 31x^{30} + 434x^{28} + 3629x^{26} + 20198x^{24} + 78938x^{22} + 222724x^{20} + 459365x^{18} \\ &\quad + 693530x^{16} + 760145x^{14} + 593801x^{12} + 320464x^{10} + 113705x^8 + 24470x^6 + 2774x^4 + 125x^2 + 1, \\ g_1 &= \tilde{\phi}(P_{32}(4, 4, 23), x) = x^{32} + 31x^{30} + 434x^{28} + 3629x^{26} + 20197x^{24} + 78917x^{22} + 222534x^{20} + 458396x^{18} \\ &\quad + 690471x^{16} + 753971x^{14} + 585871x^{12} + 314249x^{10} + 111032x^8 + 24007x^6 + 2792x^4 + 132x^2 + 1. \end{aligned}$$

So we have

$$h_1g_0 - h_0g_1 = x(x^4 + 3x^2 + 1)(x^{12} + 12x^{10} + 53x^8 + 107x^6 + 99x^4 + 34x^2 + 1) > 0 \text{ for all } x > 0.$$

By using computer we can also find

$$\mathbb{E}(H(0)) \doteq 38.616923, \quad \mathbb{E}(G(0)) \doteq 38.616742$$

So using Theorem 3.1, we have $\mathbb{E}(P_n(2, 7, n - 10)) - \mathbb{E}(P_n(4, 4, n - 9)) = \mathbb{E}(H(n - 31)) - \mathbb{E}(G(n - 31)) \geq \mathbb{E}(H(0)) - \mathbb{E}(G(0)) \doteq 0.000181 > 0$. \square

Theorem 5.6. *Let $n \geq 31$. Let $S'_n = S_n \setminus \{P_n(2, 5, n - 8), P_n(2, 3, n - 6), P_n(2, 1, n - 4)\}$ be the first $\lfloor \frac{n-9}{2} \rfloor$ trees in the quasi-order list (5.1) of S_n . Then P_n and the $\lfloor \frac{n-9}{2} \rfloor$ trees in S'_n are the first $\lfloor \frac{n-7}{2} \rfloor$ largest energy trees in the class of all trees of order n .*

Proof. It is obvious by the quasi-order list (5.1) that the smallest energy tree in the set $\{P_n\} \cup S'_n$ is $P_n(2, 7, n - 10)$. Now take any tree $T \notin \{P_n\} \cup S'_n$ of order n , we consider the following four cases:

Case 1: $T \in (C2)$. Then $T \in S_n \setminus S'_n$. By the quasi-order list (5.1) we have $T \prec P_n(2, 7, n - 10)$.

Case 2: $T \in (C3)$. Then by Theorem 5.2 and Theorem 5.5 we have

$$\mathbb{E}(T) \leq \mathbb{E}(P_n(4, 4, n - 9)) < \mathbb{E}(P_n(2, 7, n - 10)).$$

Case 3: $T \in (C4)$. Then by Theorem 5.2, 5.3 and the list (5.1) we have

$$\mathbb{E}(T) \leq \mathbb{E}(P_n(2, 2, 2, n - 7)) < \mathbb{E}(P_n(2, 1, n - 4)) < \mathbb{E}(P_n(2, 7, n - 10)).$$

Case 4: $T \in (C5)$.

Subcase 4.1: $N_3(T) = 2$ and $\Delta(T) = 3$. Then T is of the form $T_n(a, b|c, d)$. So by Theorem 4.2, 4.3, 5.4 and the list (5.1) we have

$$\mathbb{E}(T) < \mathbb{E}(P_n(2, 1, n - 4)) < \mathbb{E}(P_n(2, 7, n - 10)).$$

Subcase 4.2: $N_3(T) = 2$ and $\Delta(T) \geq 4$. Then a tree T' with $N_3(T') = 2$ and $\Delta(T') = 3$ can be obtained from T by using total edge grafting several times. So $T \prec T'$, and thus by Subcase 4.1 we have $\mathbb{E}(T) < \mathbb{E}(T') < \mathbb{E}(P_n(2, 7, n - 10))$.

Subcase 4.3: $N_3(T) \geq 3$. Using Theorem 4.1 several times we can obtain a tree T' with $N_3(T') = 2$ and $T \prec T'$. So by Subcases 4.1 and 4.2 we have $\mathbb{E}(T) < \mathbb{E}(T') < \mathbb{E}(P_n(2, 7, n - 10))$. \square

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